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Serial No.:

Title: **Carbonate Solvent For Electrolytes In Lithium and Lithium Ion Cell**

Docket No.: **CECOM 5443**

Government Interest

[001] The invention described herein may be manufactured, used, imported, sold, and licensed by or for the Government of the United States of America without the payment of any royalty thereon or therefor.

Background of the Invention

1. Field of the Invention

[002] The present invention relates generally to electrolytes for electrochemical cells and, more particularly, to organic solvents used with non-aqueous electrolytes.

2. Related Art

[003] Electrochemical cells, such as lithium batteries, may contain a non-aqueous electrolyte that includes an organic solvent. Typically, a supporting electrolyte, such as lithium hexafluorophosphate ($LiPF_6$) is dissolved in an organic solvent, e.g., a cyclic carbonate compound such as ethylene carbonate or propylene carbonate. Also, various volume ratios of low viscosity ester solvents such as diethyl carbonate and dimethyl carbonate may be used to form a solvent mixture.

[004] In one particular example of an organic solvent mixture for a battery electrolyte, U.S. Patent No. 6,566,015 describes a composition that includes at least one type each of a cyclic carbonate compound, an alkyl mono-carbonate compound, an alkylene bis-carbonate compound, a glycol diether compound and a phosphorous-containing organic compound. The use of the gycol diether compound is said to lower the internal resistance of the battery as a result of increasing the mobility of lithium ions at the solid-liquid interface. However, it has been found that this composition suffers from the drawback that it is rather complex and difficult to produce.

[005] Accordingly, it is desired to provide a relatively simple organic solvent mixture that provides for increased electrochemical cell performance properties including an increased energy density output of the cell.

Summary of the Invention

[006] In accordance with an embodiment of the present invention, an electrochemical cell comprises an anode comprising a salt, a cathode insulated from the anode and a non-aqueous electrolyte in contact with the anode. The electrolyte may comprise an organic solvent that comprises at least approximately one percent by volume trimethylene carbonate.

[007] In a more particular embodiment of the invention, the organic solvent may comprise a volume percentage of trimethylene carbonate that is greater than approximately 35%.

[008] In another embodiment, the organic solvent may further comprise dimethyl carbonate having a volume percentage that is in the range of between approximately 99% and approximately 1%.

[009] In another particular embodiment of the invention, the organic solvent comprises a volume ratio of 1:1 of trimethylene carbonate and dimethyl carbonate.

[010] In a further particular embodiment, the organic solvent may further comprise at least one material selected from the group consisting of ethylene carbonate, propylene carbonate, dimethyl carbonate, diethyl carbonate and ethyl methyl carbonate.

[011] In still a further particular embodiment, the salt may comprise at least one material from the group consisting of $LiPF_6$, $LiAsF_6$, $LiClO_4$, $LiC(SO_2CF_3)_3$, lithium triflates, lithium imides, and lithium methides.

Brief Description of the Drawings

[012] Other objects and advantages of the invention will be evident to one of ordinary skill in the art from the following detailed description made with reference to the accompanying drawings, in which:

[013] Figure 1 is a cross-sectional view of a coin-shaped battery comprising a non-aqueous electrolyte in accordance with an embodiment of the present invention;

[014] Figure 2 is a diagram showing the structure and chemical formula of trimethylene carbonate;

[015] Figure 3 is a graph showing conductivity versus temperature for two example organic solvent compositions, the first example comprising trimethylene carbonate

and the second example comprising a mixture of trimethylene carbonate and dimethyl carbonate; and

[016] Figure 4 is a graph showing potential versus capacity for an electrochemical cell including an electrolyte solution comprising a one molar $LiPF_6$ solution combined with the second example mixture of trimethylene carbonate and dimethyl carbonate.

Detailed Description of the Preferred Embodiment

[017] One embodiment of the present invention concerns an electrochemical cell or rechargeable/non-rechargeable battery that includes a cyclic organic solvent for a non-aqueous electrolyte. The organic solvent may comprise trimethylene carbonate ($C_4H_6O_3$) that has a relatively high dielectric constant. It has been found that an especially high energy density output may be attained from a battery containing a non-aqueous electrolyte with such an organic solvent.

[018] Referring now to Figure 1, an electrochemical cell, comprising a non-aqueous electrolyte in accordance with one embodiment of the present invention, is illustrated generally at 10. In this embodiment, the electrochemical cell or battery 10 comprises a negative electrode case 12 and a positive electrode case 14 that are interconnected by an insulating gasket 16 composed of, e.g., polypropylene. It will be recognized that the battery 10 is shown for illustrational purposes only and, e.g., may be rechargeable or non-rechargeable and may function as a primary or secondary cell in accordance with the present invention.

[019] The negative electrode case 12 may be composed of a stainless steel and is in contact with a cathode 18 that comprises a negative collector 20 and a negative

charge body 22. The negative collector 20 may be composed of copper and the negative charge body 22 may be composed of carbon powder.

[020] The positive electrode case 14, similar to the negative electrode case 12, may also be formed of a stainless steel and is in contact with an anode 24 that comprises a positive collector 26 and a positive charge body 28. The positive collector 26 may be composed of aluminum and the positive charge body 28 may be composed of a lithium compound such as $LiCoO_2$.

[021] A separator 30, composed of an insulating material, may be disposed between the cathode 18 and the anode 24 and a non-aqueous electrolyte 32, as described in more detail below, may be located in contact with the positive electrode.

[022] The electrolyte 32 comprises a lithium salt and is preferably lithium hexafluorophosphate ($LiPF_6$), although, other lithium salts may be used such as, but not limited to, $LiPF_6$, $LiAsF_6$, $LiClO_4$, $LiC(SO_2CF_3)_3$, lithium triflates, lithium imides, and lithium methides. It will be appreciated that other lithium compounds including lithium ions, lithium alloys and lithium polymers may be employed in accordance with the present invention.

[023] In accordance with a feature of this embodiment, the electrolyte 32 also comprises an organic solvent that is preferably trimethylene carbonate ($C_4H_6O_3$), the chemical structure and formula of which are shown generally at 34 in Figure 2. The organic solvent may comprise a volume percentage of trimethylene carbonate that is at least 1% and may be greater than 35%. The solvent properties of trimethylene carbonate are shown in the following Table.

TABLE

Solvent	Boiling Point, °C	Freezing Point, °C	Dielectric Constant, ε_{50}, D
Trimethylene Carbonate, ($C_4H_6O_3$)	120	45	73

[024] It will be understood that the electrolyte 32 may also comprise an organic solvent mixture comprising trimethylene carbonate and one or more other organic solvents. For example, it has been found that a solvent mixture of trimethylene carbonate and dimethyl carbonate in a 1:1 volume ratio is most preferable, although, other ratios are contemplated. When employed in a solvent mixture, the volume percentage of dimethyl carbonate may range between approximately 99% and approximately 1%. Solvents that may be combined with trimethylene carbonate in the practice of the present invention include, but are not limited to, ethylene carbonate, propylene carbonate, dimethyl carbonate, diethyl carbonate, and ethyl methyl carbonate.

[025] Referring now to Figure 3, the conductivity versus temperature (°C) for two example non-aqueous electrolyte solutions are shown. In a first example, a one mole/liter salt solution of lithium hexafluorophosphate ($LiPF_6$) is mixed with trimethylene carbonate having a solvent volume percentage of 100% and, in a second example, a one mole/liter solution of lithium hexafluorophosphate ($LiPF_6$) is mixed with 1:1 volume ratio binary mixture of trimethylene carbonate and dimethyl carbonate the latter having a solvent volume percentage of 50%.

[026] Figure 4 illustrates the potential versus capacity for an electrochemical cell that has a positive collector that contains $LiCoO_2$ and comprises an electrolyte solution provided in the second example described above. The cell was cycled at one half (.5) mA/cm^2 between 4.15 and 2.5 volts. While one molar salt solutions are illustrated herein, it will be recognized that higher or lower concentrations of salt may be employed to optimize the solution conductivity and overall cell performance.

[026] While the present invention has been described in connection with what are presently considered to be the most practical and preferred embodiments, it is to be understood that the present invention is not limited to these herein disclosed embodiments. Rather, the present invention is intended to cover all of the various modifications and equivalent arrangements included within the spirit and scope of the appended claims.